```
=> fil reg; d stat que l4
FILE 'REGISTRY' ENTERED AT 12:01:24 ON 27 OCT 92
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STRUCTURE FILE UPDATES:  23 OCT 92   HIGHEST RN 144124-63-0
DICTIONARY FILE UPDATES: 26 OCT 92   HIGHEST RN 144124-63-0


L2                STR
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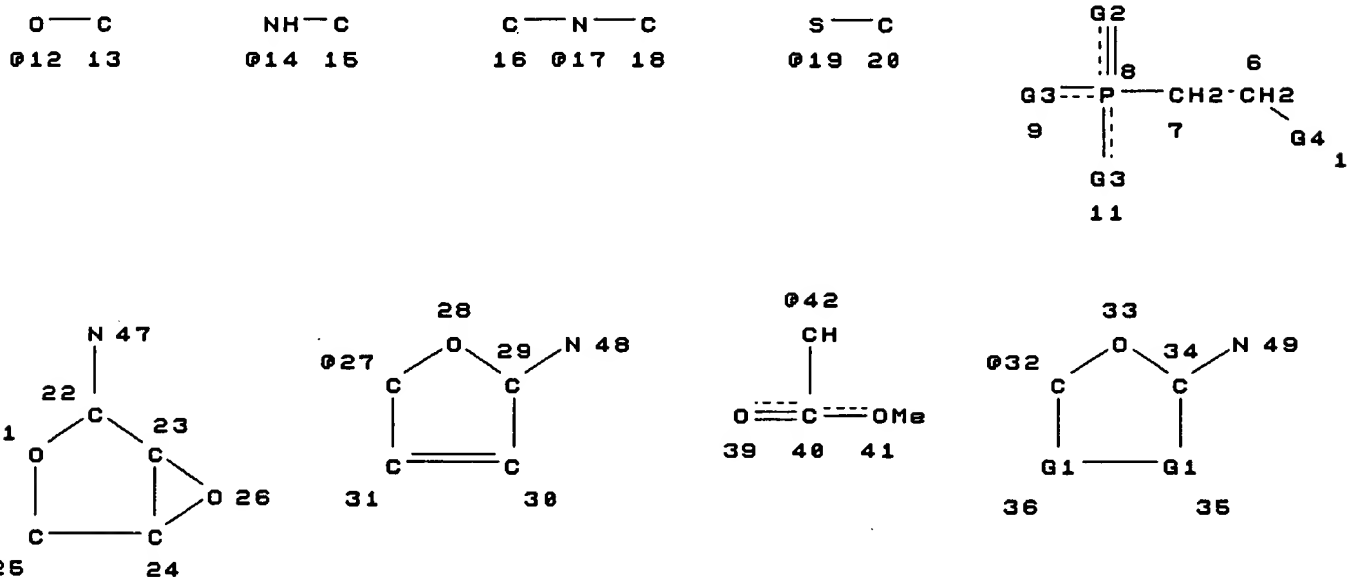


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VAR G3=OH/NH2/SH/12/14/17/19
VAR G4=25/27/32
NODE ATTRIBUTES:
NSPEC    IS R  } ring node  AT  47
NSPEC    IS R  }            AT  48
NSPEC    IS R  }            AT  49

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  43
L4            34 SEA FILE=REGISTRY SSS FUL L2

100.0% PROCESSED    289 ITERATIONS                    34 ANSWERS
SEARCH TIME: 00.00.10


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1          RN             142574-81-0  REGISTRY
2          RN             142574-77-4  REGISTRY
3          RN             142574-76-3  REGISTRY
4          RN             142574-75-2  REGISTRY
5          RN             137248-62-5  REGISTRY
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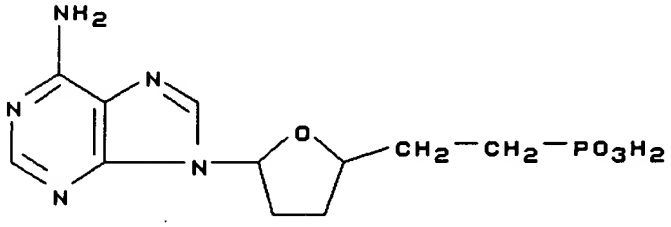
6	RN	137248-58-9	REGISTRY
7	RN	137104-27-9	REGISTRY
8	RN	137104-26-8	REGISTRY
9	RN	137104-25-7	REGISTRY
10	RN	127235-91-0	REGISTRY
11	RN	127235-90-9	REGISTRY
12	RN	127235-81-8	REGISTRY
13	RN	127235-80-7	REGISTRY
14	RN	124685-23-0	REGISTRY
15	RN	124685-22-9	REGISTRY
16	RN	124572-53-8	REGISTRY
17	RN	124572-52-7	REGISTRY
18	RN	117544-95-3	REGISTRY
19	RN	117513-96-9	REGISTRY
20	RN	69124-08-9	REGISTRY
21	RN	52663-96-4	REGISTRY
22	RN	47351-06-4	REGISTRY
23	RN	34393-67-4	REGISTRY
24	RN	34295-89-1	REGISTRY
25	RN	34295-88-0	REGISTRY
26	RN	34212-86-7	REGISTRY
27	RN	34212-85-6	REGISTRY
28	RN	31198-98-8	REGISTRY
29	RN	31087-99-7	REGISTRY
30	RN	31087-98-6	REGISTRY
31	RN	31080-13-4	REGISTRY
32	RN	25203-85-4	REGISTRY
DR	25204-02-8		
33	RN	22257-15-4	REGISTRY
DR	25204-03-9		
34	RN	7307-92-8	REGISTRY

=> d ide can l4 1 5 7 10 14 16 18-24 26 28 29 31-34

L4 ANSWER 1 OF 34 COPYRIGHT 1992 ACS
RN 142574-81-0 REGISTRY
CN Phosphonic acid, [2-[5-(6-amino-9H-purin-9-yl)tetrahydro-2-furanyl]ethyl]-, calcium salt (1:1), (2S-cis)- (9CI) (CA INDEX NAME)
MF C11 H16 N5 O4 P . Ca
SR CA
LC CA
DES *

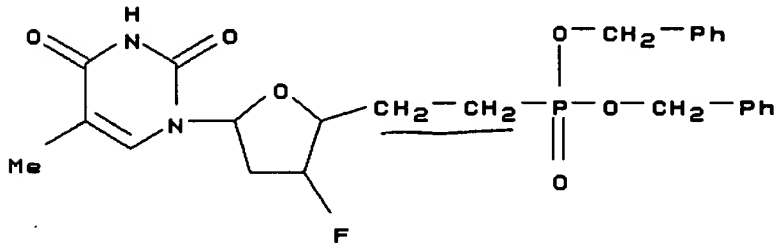


• Ca

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA117(7):70237r

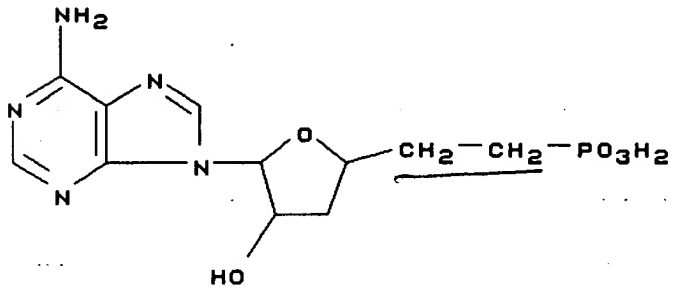
L4 ANSWER 5 OF 34 COPYRIGHT 1992 ACS
RN 137248-62-5 REGISTRY
CN Phosphonic acid, [2-[5-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-3-fluorotetrahydro-2-furanyl]ethyl]-, bis(phenylmethyl) ester, [2R-(2.alpha.,3.beta.,5.alpha.)]- (9CI) (CA INDEX NAME)
MF C25 H28 F N2 O6 P
SR CA
LC CA
DES 1:2R2:2A,3B,5A



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA115(23):256521t

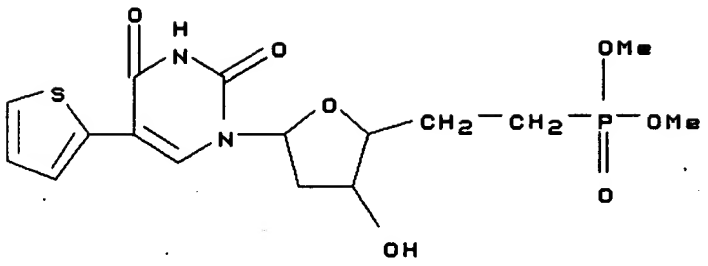
L4 ANSWER 7 OF 34 COPYRIGHT 1992 ACS
RN 137104-27-9 REGISTRY
CN 9H-Purin-6-amine, 9-(3,5,6-trideoxy-6-phosphono-.beta.-D-erythro-hexofuranosyl)- (9CI) (CA INDEX NAME)
MF C11 H16 N5 O5 P
SR CA
LC CA
DES 5:B-D-ERYTHRO



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA115(21):232734p

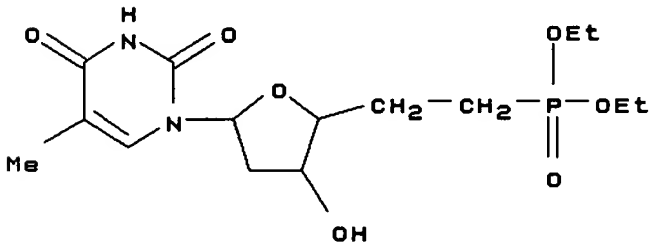
L4 ANSWER 10 OF 34 COPYRIGHT 1992 ACS
RN 127235-91-0 REGISTRY
CN 2,4(1H,3H)-Pyrimidinedione, 5-(2-thienyl)-1-[2,5,6-trideoxy-6-(dimethoxyphosphinyl)-.beta.-D-erythro-hexofuranosyl]- (9CI) (CA INDEX NAME)
MF C16 H21 N2 O7 P S
SR CA
LC CA
DES 5:B-D-ERYTHRO



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P CA112(25):235778e

L4 ANSWER 14 OF 34 COPYRIGHT 1992 ACS
RN 124685-23-0 REGISTRY
CN 2,4(1H,3H)-Pyrimidinedione, 5-methyl-1-[2,5,6-trideoxy-6-(diethoxyphosphinyl)-.beta.-D-threo-hexofuranosyl]- (9CI) (CA INDEX NAME)
MF C15 H25 N2 O7 P
SR CA
LC CA, CASREACT
DES 5:B-D-THREO

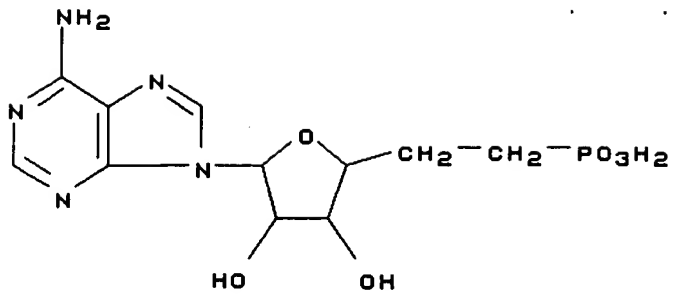


2 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA116(23):236116g

REFERENCE 2: CA112(7):56529c

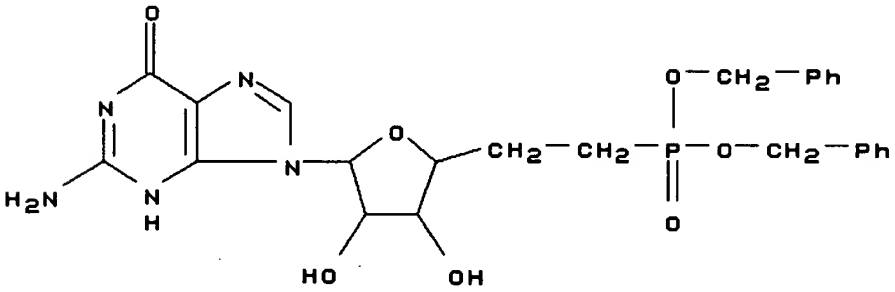
L4 ANSWER 16 OF 34 COPYRIGHT 1992 ACS
RN 124572-53-8 REGISTRY
CN 9H-Purin-6-amine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-, monoammonium salt (9CI) (CA INDEX NAME)
MF C11 H16 N5 O6 P . H3 N
SR CA
LC CA, CASREACT
DES 5:B-D-RIBO
CRN (22257-15-4)



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA112(5):36339n

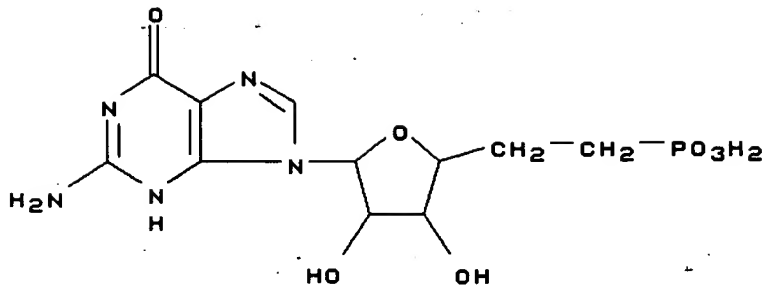
L4 ANSWER 18 OF 34 COPYRIGHT 1992 ACS
RN 117544-95-3 REGISTRY
CN 6H-Purin-6-one, 2-amino-9-[6-[bis(phenylmethoxy)phosphinyl]-5,6-dideoxy-.beta.-D-ribo-hexofuranosyl]-1,9-dihydro- (9CI) (CA INDEX NAME)
MF C25 H28 N5 O7 P
SR CA
LC CA, CASREACT
DES 5:B-D-RIBO



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA109(25):231447m

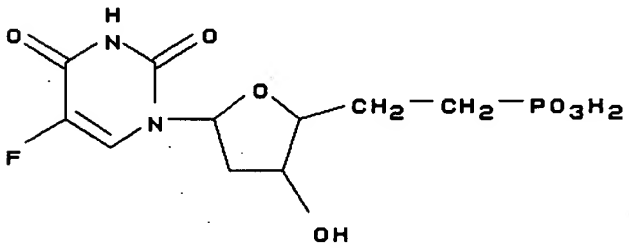
L4 ANSWER 19 OF 34 COPYRIGHT 1992 ACS
RN 117513-96-9 REGISTRY
CN 6H-Purin-6-one, 2-amino-9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-1,9-dihydro- (9CI) (CA INDEX NAME)
MF C11 H16 N5 O7 P
SR CA
LC CA, CASREACT
DES 5:B-D-RIBO

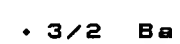


1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA109(25):231447m

L4 ANSWER 20 OF 34 COPYRIGHT 1992 ACS
RN 69124-08-9 REGISTRY
CN 2,4(1H,3H)-Pyrimidinedione, 5-fluoro-1-(2,5,6-trideoxy-6-phosphono-.beta.-D-erythro-hexofuranosyl)-, barium salt (1:1) (9CI) (CA INDEX NAME)
MF C10 H14 F N2 O7 P . 3/2 Ba
LC CA
DES *

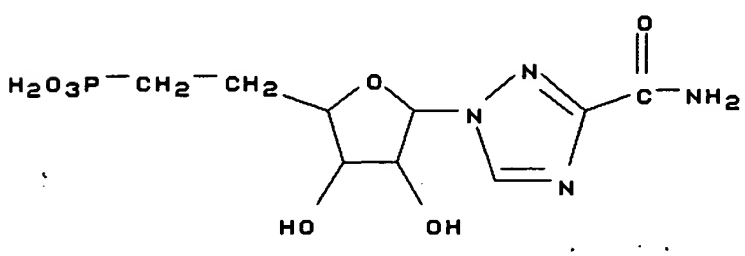




1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA90(13):97373t

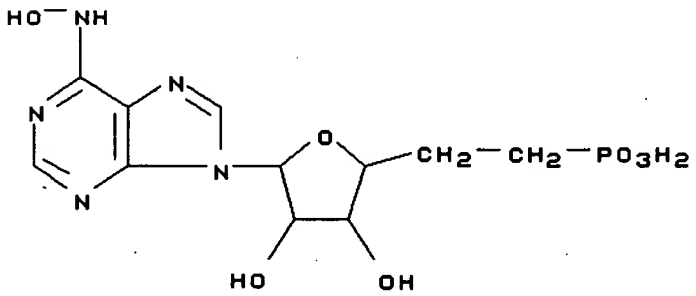
L4 ANSWER 21 OF 34 COPYRIGHT 1992 ACS
RN 52663-96-4 REGISTRY
CN 1H-1,2,4-Triazole-3-carboxamide, 1-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (9CI) (CA INDEX NAME)
MF C9 H15 N4 O7 P
LC BEILSTEIN, CA
DES 5:B-D-RIBO



1 REFERENCES IN FILE CA (1967 TO DATE)

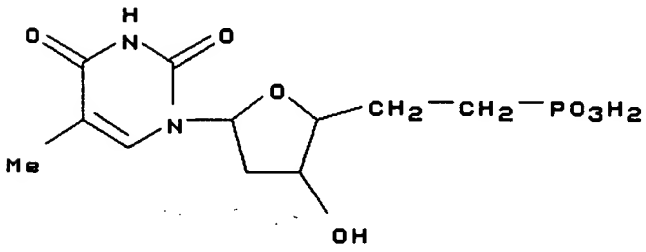
REFERENCE 1: CA81(19):114436z

L4 ANSWER 22 OF 34 COPYRIGHT 1992 ACS
RN 47351-06-4 REGISTRY
CN 6H-Purin-6-one, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-1,9-dihydro-, oxime (9CI) (CA INDEX NAME)
MF C11 H16 N5 O7 P
CI COM
DES 5:B-D-RIBO



0 REFERENCES IN FILE CA (1967 TO DATE)

L4 ANSWER 23 OF 34 COPYRIGHT 1992 ACS
RN 34393-67-4 REGISTRY
CN Thymine, 1-(2,5,6-trideoxy-6-phosphono-.beta.-D-erythro-hexofuranosyl)- (8CI) (CA INDEX NAME)
MF C11 H17 N2 O7 P
CI COM
LC CA, IFICDB, IFIPAT, IFIUDB
DES 5:B-D-ERYTHRO



1 REFERENCES IN FILE CA (1967 TO DATE)

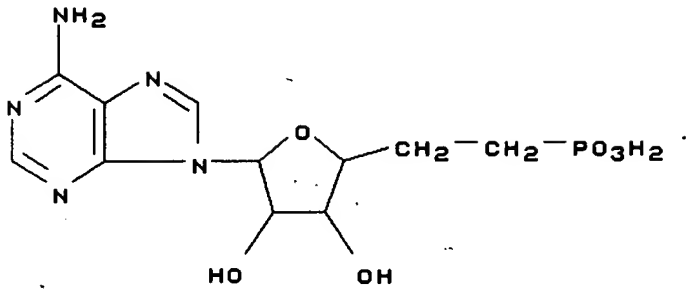
REFERENCE 1: P CA75(21):130083p

L4 ANSWER 24 OF 34 COPYRIGHT 1992 ACS
RN 34295-89-1 REGISTRY
CN Adenine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-, compd. with triethylamine (1:2) (8CI) (CA INDEX NAME)
MF C11 H16 N5 O6 P . 2 C6 H15 N
LC CA

CM 1

CRN 22257-15-4
CMF C11 H16 N5 O6 P

CDES 5:B-D-RIBO



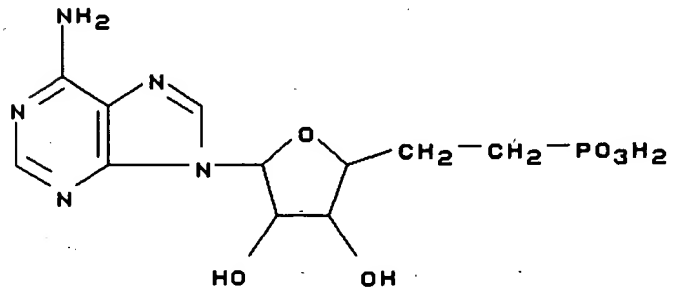
CM 2

CRN 121-44-8
CMF C6 H15 N

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P CA75(19):118548m

L4 ANSWER 26 OF 34 COPYRIGHT 1992 ACS
RN 34212-86-7 REGISTRY
CN 9H-Purin-6-amine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-, disodium salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-, disodium salt (8CI)
MF C11 H16 N5 O6 P . 2 Na
LC CA, IFICDB, IFIPAT, IFIUDB
DES 5:B-D-RIBO
CRN (22257-15-4)



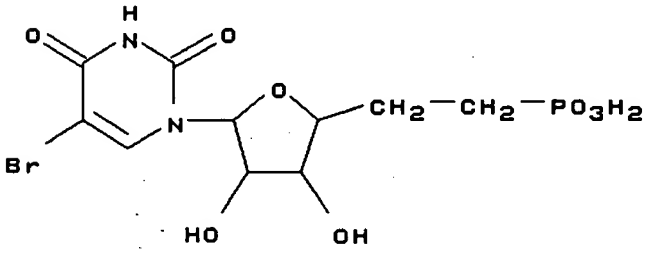
3 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA97(1):2705k

REFERENCE 2: P CA75(21):130083p

REFERENCE 3: P CA75(19):118548m

L4 ANSWER 28 OF 34 COPYRIGHT 1992 ACS
RN 31198-98-8 REGISTRY
CN Uracil, 5-bromo-1-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (8CI) (CA INDEX NAME)
MF C10 H14 Br N2 O8 P
LC CA, IFICDB, IFIPAT, IFIUDB
DES 5:B-D-RIBO



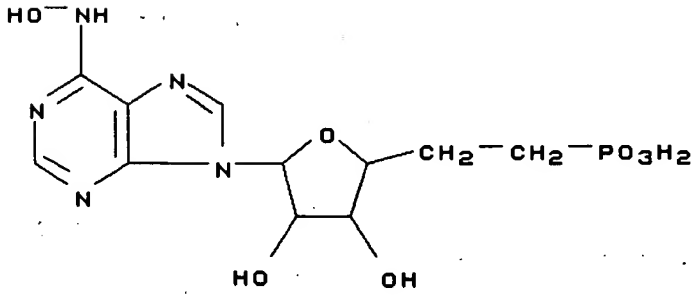
1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P CA74(11):54150v

L4 ANSWER 29 OF 34 COPYRIGHT 1992 ACS
RN 31087-99-7 REGISTRY
CN Adenine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-N-hydroxy-, compd. with triethylamine (8CI) (CA INDEX NAME)
MF C11 H16 N5 O7 P . x C6 H15 N
LC CA, IFICDB, IFIPAT, IFIUDB

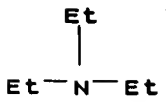
CM 1

CRN 47351-06-4
CMF C11 H16 N5 O7 P
CDES 5:B-D-RIBO



CM 2

CRN 121-44-8
CMF C6 H15 N



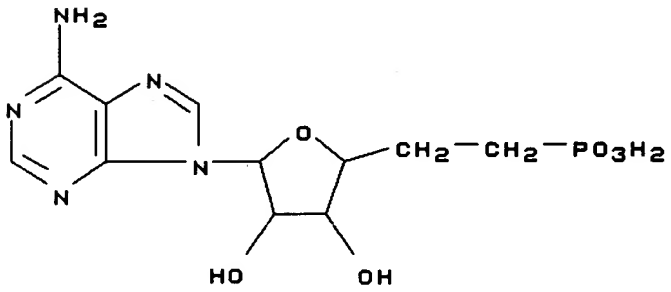
1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P CA74(11):54150v

L4 ANSWER 31 OF 34 COPYRIGHT 1992 ACS
RN 31080-13-4 REGISTRY
CN Adenine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)-, compd. with triethylamine (8CI) (CA INDEX NAME)
MF C11 H16 N5 O6 P . x C6 H15 N
LC CA, IFICDB, IFIPAT, IFIUDB

CM 1

CRN 22257-15-4
CMF C11 H16 N5 O6 P
CDES 5:B-D-RIBO



CM 2

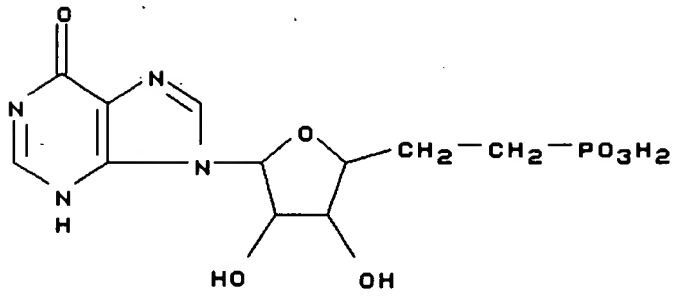
CRN 121-44-8
CMF C6 H15 N

1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: P CA74(11):54150v

L4 ANSWER 32 OF 34 COPYRIGHT 1992 ACS
RN 25203-85-4 REGISTRY
CN 6H-Purin-6-one, 9-(5,6-dideoxy-6-O-phosphono-.beta.-D-ribo-hexofuranosyl)-1,9-dihydro- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Hypoxanthine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (8CI)
OTHER NAMES:

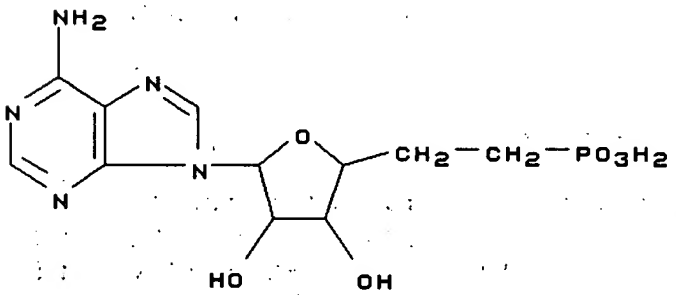
CN 6′-Deoxyhomoinosine 6′-phosphonic acid
DR 25204-02-8
MF C11 H15 N4 O7 P
LC CA
DES 5:B-D-RIBO



1 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA73(1):437e

L4 ANSWER 33 OF 34 COPYRIGHT 1992 ACS
RN 22257-15-4 REGISTRY
CN 9H-Purin-6-amine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenine, 9-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (8CI)
OTHER NAMES:
CN 5′-Deoxy-5′-homoadenosine phosphonic acid
CN 6′-Deoxyhomoadenosine 6′-phosphonic acid
CN ACP
DR 25204-03-9
MF C11 H16 N5 O6 P
CI COM
LC BEILSTEIN, CA, CASREACT, CJACS, IFICDB, IFIPAT, IFIUDB
DES 5:B-D-RIBO



18 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA113(13):111903t

REFERENCE 2: CA108(21):187168z

REFERENCE 3: CA108(19):167857v

REFERENCE 4: CA107(21):193874x

REFERENCE 5: CA107(21):190370u

REFERENCE 6: CA106(3):12328h

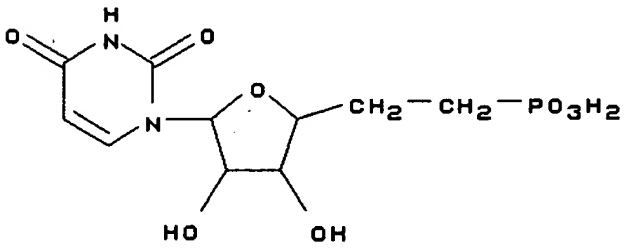
REFERENCE 7: CA105(11):97866j

REFERENCE 8: CA102(21):181349p

REFERENCE 9: CA98(17):137998z

REFERENCE 10: CA92(15):122602t

L4 ANSWER 34 OF 34 COPYRIGHT 1992 ACS
RN 7307-92-8 REGISTRY
CN 2,4(1H,3H)-Pyrimidinedione, 1-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Uracil, 1-(5,6-dideoxy-6-phosphono-.beta.-D-ribo-hexofuranosyl)- (7CI, 8CI)
MF C10 H15 N2 O8 P
CI COM
LC BEILSTEIN, CA, CAOLD, CASREACT, IFICDB, IFIPAT, IFIUDB
DES 5:B-D-RIBO



REFERENCES IN FILE CAOLD (PRIOR TO 1967)
6 REFERENCES IN FILE CA (1967 TO DATE)

REFERENCE 1: CA108(21):187168z

REFERENCE 2: CA108(19):167857v

REFERENCE 3: P CA75(21):130083p

REFERENCE 4: P CA75(19):118548m

REFERENCE 5: P CA74(11):54150v

REFERENCE 6: CA70(1):4503j

=> fil ca; d que 15
FILE 'CA' ENTERED AT 12:04:44 ON 27 OCT 92
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FILE COVERS 1967 -17 Oct 92 (921017/ED) VOL 117 ISS 16.
For OFFLINE Prints or Displays, use the ABS or ALL formats to obtain abstract graphic structures. The AB format DOES NOT display structure diagrams.

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L2              STR
L4           34 SEA FILE=REGISTRY SSS FUL L2
L5           32 SEA FILE=CA L4 OR L4/D
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=> d bib abs hit l5 1-32
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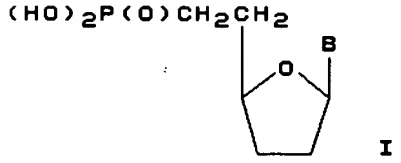
L5 ANSWER 1 OF 32 COPYRIGHT 1992 ACS
AN CA117(7):70237r
TI Syntheses of phosphonate analogs of dideoxyadenosine (DDA)-, dideoxycytidine (DDC)-, dideoxyinosine (DDI)-, and deoxythymidine (DDT)-5′-monophosphates
AU Secrist, John A., III; Riggs, Robert M.; Comber, Robert N.; Montgomery, John A.
CS Org. Chem. Res. Dep., South. Res. Inst.
LO Birmingham, AL 35255-5305, USA
SO Nucleosides Nucleotides, 11(2-4), 947-56
SC 33-9 (Carbohydrates)
DT J
CO NUNUD5
IS 0732-8311
PY 1992
LA Eng
AN CA117(7):70237r
GI

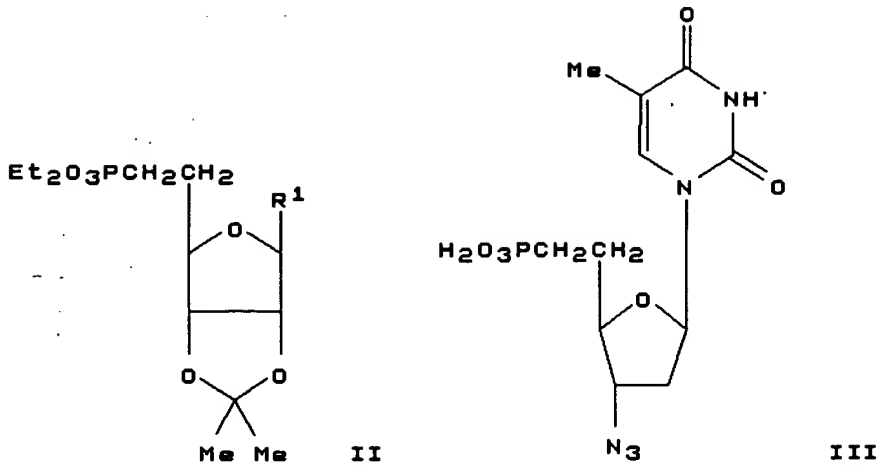


I

AB Phosphonate derivs. I of ddA, ddC, ddI and ddT were prepd. by condensing the 5′-aldehydes with (PhO)2P(O)CH:PPh3, reducing the resultant olefins and hydrolyzing the phosphonate Ph esters, sequentially, with base and then C. atrox phosphodiesterase.
IT 142574-75-2P 142574-76-3P 142574-77-4P
142574-81-0P
(prepn. of)

L5 ANSWER 2 OF 32 COPYRIGHT 1992 ACS
AN CA116(23):236116g
TI New synthesis of sugar, nucleoside and .alpha.-amino acid phosphonates
AU Barton, Derek H. R.; Gero, Stephane D.; Quiclet-Sire, Beatrice; Samadi, Mohammad
CS Dep. Chem., Texas A and M Univ.
LO College Station, TX 77843, USA
SO Tetrahedron, 48(9), 1627-36
SC 34-2 (Amino Acids, Peptides, and Proteins)
SX 33
DT J
CO TETRAB
IS 0040-4020
PY 1992
LA Eng
OS CASREACT 116:236116

AN CA116(23):236116g
GI

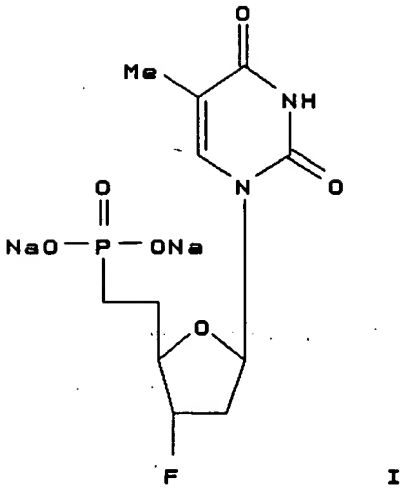


II III

AB Photolysis of N-hydroxy-2-thiopyridone esters derived from uronic acids or .alpha.-amino acids in presence of vinyl phosphonate affords the corresponding phosphonate derivs. Thus, in situ esterification of protected amino acids Boc-X-OCH2Ph (Boc = Me3CO2C; X = Asp, Glu) with N-hydroxy-2-thiopyridone followed by radical addn. with H2C:CHPO3Et2 gave phosphonates Boc-L-NHCH(CO2CH2Ph)(CH2)nCHRPO3Et2 (I; n = 2, 3; R = 2-pyridylthio). Removal of the thiopyridyl groups in I with Bu3SnH gave phosphonic acid analogs I (R = H). Sugar and nucleoside phosphonates II (R1 = OMe, protected adenine, uracil) were prepd. similarly. A convenient route for the synthesis of III, the isostere of AZT-5′ monophosphate, is described.

IT 124685-23-0P
(prepn. and mesylation of)

L5 ANSWER 3 OF 32 COPYRIGHT 1992 ACS
AN CA115(23):256521t
TI Synthesis of a phosphonomethyl analog of 3′-deoxy-3′-fluorothymidine
AU Almer, Helena; Classon, Bjoern; Samuelsson, Bertil; Kvarnstroem, Ingemar
CS Dep. Org. Chem., Stockholm Univ.
LO Stockholm S-106 91, Swed.
SO Acta Chem. Scand., 45(7), 766-7
SC 33-9 (Carbohydrates)
DT J
CO ACHSE7
IS 0904-213X
PY 1991
LA Eng
AN CA115(23):256521t
GI



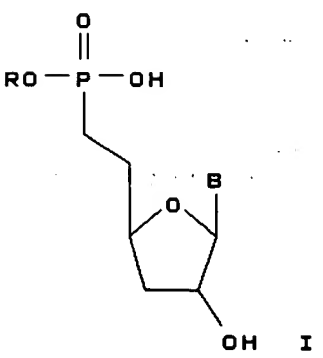
I

AB Phosphonomethyldeoxyfluorothymidine I was prepd. from 1-(2′,3′-dideoxy-3′-fluoro-.beta.-D-erythro-pentofuranosyl)thymine in 6 steps. I showed any significant anti-HIV activity.

IT 137248-58-9P
(prepn. and antiviral activity of)

IT 137248-62-5P
(prepn. and sequential hydrogenation and sapon. of)

L5 ANSWER 4 OF 32 COPYRIGHT 1992 ACS
AN CA115(21):232734p
TI Synthesis of some 3′,5′-dideoxy-5′-C-phosphonomethyl nucleosides
AU Ioannidis, Panagiotis; Classon, Bjoern; Samuelsson, Bertil; Kvarnstroem, Ingemar
CS Dep. Org. Chem., Stockholm Univ.
LO Stockholm S-106 91, Swed.
SO Acta Chem. Scand., 45(7), 746-50
SC 33-9 (Carbohydrates)
SX 1
DT J
CO ACHSE7
IS 0904-213X
PY 1991
LA Eng
OS CASREACT 115:232734
AN CA115(21):232734p
GI



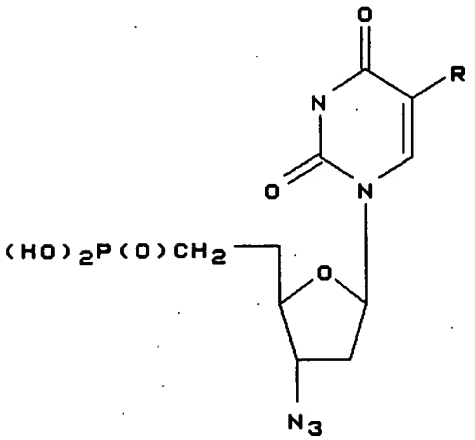
I

AB Title compds. I (B = thymine, cytosine, R = NH4; B = adenine, R = H) have been synthesized and tested for anti-HIV activity. The key

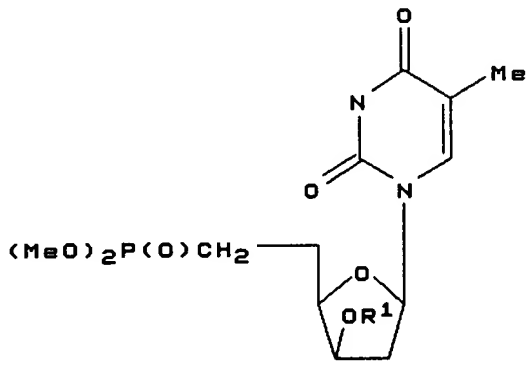
steps involved an Arbuzov reaction between (EtO)3P and 3,5,6-trideoxy-6-iodo-1,2-O-isopropylidene-.alpha.-D-erythro-hexofuranose, followed by condensation with the appropriate nucleoside bases.

IT 137104-25-7P 137104-26-8P 137104-27-9P
(prepn. and antiviral activity of)

L5 ANSWER 5 OF 32 COPYRIGHT 1992 ACS
AN CA114(13):122988w
TI Preparation of virucidal 3′-deoxy-3′-azidonucleoside 5′-phosphonic acids
AU Miyasaka, Sada; Tanaka, Hiromichi
CS Mitsubishi Kasei Corp.
LO Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
PI JP 02262588 A2 25 Oct 1990 Heisei
AI JP 89-84298 3 Apr 1989
IC ICM C07H019-073
ICA A61K031-70
SC 33-9 (Carbohydrates)
SX 1
DT P
CO JKXXAF
PY 1990
LA Japan
OS MARPAT 114:122988
AN CA114(13):122988w
GI



I



II

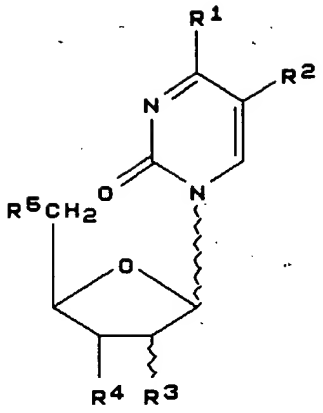
AB Title compds. I (R = H, C1-4 alkyl) and their pharmacol. acceptable salts, useful as virucides for retrovirus (e.g. human immunodeficiency virus) (no data), are prepd. Treatment of 209 mg thymidine analog II (R1 = H) (prepn. given) with mesyl chloride and p-dimethylaminopyridine in pyridine at 0.degree. for 7 h gave 345 mg II (R1 = mesyl), which was treated with NaN3 in DMF at 80.degree. for 17 h to afford 165 mg I (R = Me) di-Me ester. NaBr was treated with Me3SiCl in DMF at 40.degree. for 5 min, treated with 110 mg I (R = Me) di-Me ester at 40.degree. for 5 h, and the product was chromatographed on Dowex 50 .times. 8 (Na-type) to give 107 mg I (R = Me) di-Na salt.

IT 124685-22-9P

(prepn. and mesylation of)

L5 ANSWER 6 OF 32 COPYRIGHT 1992 ACS
AN CA113(13):111903t
TI Polynucleotide phosphorylase forms polymers from an ADP analog in which the 5′ oxygen is replaced by a methylene group
AU Breaker, R. R.; Gough, G. R.; Gilham, P. T.
CS Dep. Biol. Sci., Purdue Univ.
LO West Lafayette, IN 47907, USA
SO Nucleic Acids Res., 18(10), 3085-6
SC 9-14 (Biochemical Methods)
SX 7
DT J
CO NARHAD
IS 0305-1048
PY 1990
LA Eng
AN CA113(13):111903t
AB The synthesis of polymers of a ADP analog with phosphodiester linkages resistant to cleavage (contg. a methylene group in place of the 5′ O) is presented. Synthesis of ADP and ATP analogs and polymn. of the ADP analog are described.
IT 22257-15-4
(condensation of, with pyrophosphate)

L5 ANSWER 7 OF 32 COPYRIGHT 1992 ACS
AN CA112(25):235778e
TI Preparation of pyrimidine nucleosides as virucides and their intermediates
AU Johansson, K. Nils Gunnar; Malmberg, Hans C. G.; Noreen, Rolf; Sahlberg, S. Christer; Sohn, Daniel D.; Gronowitz, Salo
CS Medivir AB
LO Swed.
SO PCT Int. Appl., 57 pp.
PI WO 8912061 A1 14 Dec 1989
DS W: AU, DK, FI, HU, JP, KR, NO, US
AI WO 89-SE322 7 Jun 1989
PRAI SE 88-2173 10 Jun 1988
IC ICM C07H019-06
ICS C07H019-10; C07H019-24; A61K031-70; C07D239-47; C07D239-54; C07D401-04; C07D403-04; C07D405-04; C07D409-04; C07D421-04
SC 33-9 (Carbohydrates)
SX 1
DT P
CO PIXXD2
PY 1989
LA Eng
OS MARPAT 112:235778
AN CA112(25):235778e
GI



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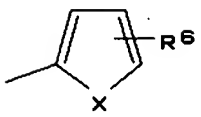
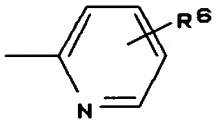
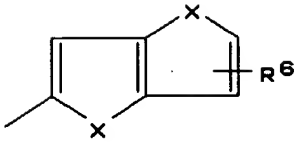
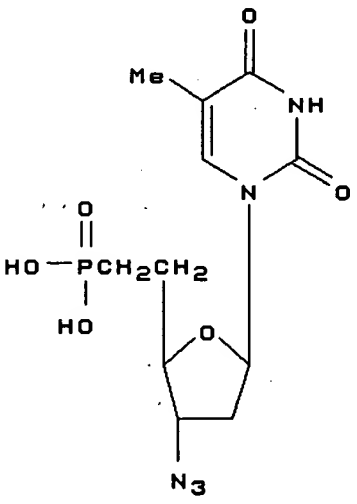
Q=  Q1=  Q2= 

AB The title compds. [I; R1 = OH, NH2; R2 = (hetero)aryl, e.g. Q-Q2; X = O, S, Se, (un)substituted NH; R3 = H, OH, F, OMe; R4 = H, F, OH or its ether or ester residue, OMe, cyano, C.tplbond.CH, N3; R5 = OH or its ether or ester residue, (CH2)nP(O)(OM)2, (CH2)nP(O)(OM)CH2P(O)(OM)2; R6 = H, straight or branched C1-10 alkyl, halo, etc.; M = H, a pharmaceutically acceptable counterion; n = 0, 1], useful for treatment of infections by viruses requiring reverse transcriptase for replication, e.g. human immunodeficiency virus (HIV) and hepatitis B virus, were prepd. Thus, silylation of 5-(2-thienyl)uracil (II) with hexamethyldisilazane in the presence of Me3SiCl and (NH4)2SO4 under reflux gave bis-trimethylsilylated II which was stirred overnight with 2-deoxy-3,5-di-O-p-toluoyl-D-ribofuranosyl chloride in ClCH2CH2Cl in the presence of mol. sieve 4A. The product was treated with MeONa in MeOH to give .alpha.- and .beta.-I (R1 = R4 = R5 = OH, R2 = 2-thienyl, R3 = H). .alpha.-I in vitro showed IC50 of 0.05-10 .mu.M against HIV in H9 cells. Analogously prepd. and tested were addnl. 26 I. Cellular toxicity of I on H9 and F500 cells and inhibition of enzymes (e.g. HIV reverse transcriptase, hepatitis B virus DNA polymerase, and herpes simplex virus type 2 DNA polymerase) by I were also given.

IT 32780-06-6P 55625-98-4P 56817-26-6P 56817-28-8P 102717-29-3P
127235-38-5P 127235-39-6P 127235-40-9P 127235-41-0P
127235-42-1P 127235-43-2P 127235-44-3P 127235-45-4P
127235-46-5P 127235-47-6P 127235-48-7P 127235-49-8P
127235-50-1P 127235-51-2P 127235-52-3P 127235-53-4P
127235-54-5P 127235-55-6P 127235-56-7P 127235-57-8P
127235-58-9P 127235-59-0P 127235-60-3P 127235-61-4P
127235-82-9P 127235-83-0P 127235-84-1P 127235-85-2P
127235-86-3P 127235-87-4P 127235-88-5P 127235-89-6P
127235-90-9P 127235-91-0P 127235-92-1P
127235-93-2P 127235-94-3P 127235-95-4P 127235-96-5P
127235-97-6P 127235-98-7P 127235-99-8P 127236-00-4P
127236-01-5P 127236-02-6P 127236-03-7P 127236-04-8P
127236-05-9P 127236-06-0P 127236-07-1P 127236-08-2P
127236-09-3P 127236-10-6P 127236-11-7P 127236-12-8P
127236-13-9P 127236-14-0P 127236-15-1P 127236-16-2P
127236-17-3P 127236-18-4P 127236-19-5P 127236-20-8P
127236-21-9P 127236-22-0P 127236-23-1P 127236-24-2P
127236-25-3P 127236-26-4P 127261-06-7P 127261-07-8P
127306-45-0P 127306-46-1P 127306-47-2P 127308-80-9P
(prepn. and reaction of, in prepn. of pyrimidine nucleoside

virucide)
IT 89647-09-6P 89647-10-9P 92233-50-6P 127235-62-5P
127235-63-6P 127235-64-7P 127235-65-8P 127235-66-9P
127235-67-0P 127235-68-1P 127235-69-2P 127235-70-5P
127235-71-6P 127235-72-7P 127235-73-8P 127235-74-9P
127235-75-0P 127235-76-1P 127235-77-2P 127235-78-3P
127235-79-4P 127235-80-7P 127235-81-8P
127282-38-6P 127306-44-9P
(prepn. of, as virucide)

L5 ANSWER 8 OF 32 COPYRIGHT 1992 ACS
AN CA112(7):56529c
TI Cleavage of a nucleosidic oxetane with carbanions: synthesis of a highly promising candidate for anti-HIV agents. A phosphonate isostere of AZT 5′-phosphate
AU Tanaka, Hiromichi; Fukui, Mariko; Haraguchi, Kazuhiro; Masaki, Mariko; Miyasaka, Tadashi
CS Sch. Pharm. Sci., Showa Univ.
LO Tokyo 142, Japan
SO Tetrahedron Lett., 30(19), 2567-70
SC 33-9 (Carbohydrates)
SX 1, 15
DT J
CO TELEAY
IS 0040-4039
PY 1989
LA Eng
OS CASREACT 112:56529
AN CA112(7):56529c
GI



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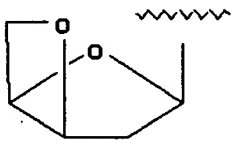
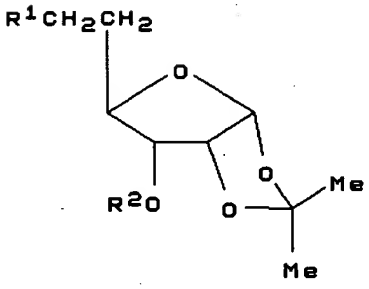


II

AB A phosphonate analog I of 3′-azido-3′-deoxythymidine (AZT) 5′-phosphate was synthesized via nucleophilic ring-opening of a nucleosidic oxetane II with (RO)2POCH2Li (R = Me, Et) as a key reaction step.
IT 124685-22-9P 124685-23-0P
(prepn. and mesylation of)

L5 ANSWER 9 OF 32 COPYRIGHT 1992 ACS

AN CA112(5):36339n
TI Use of 5-deoxy-ribo-hexofuranose derivatives for the preparation of 5′-nucleotide phosphonates and homoribonucleosides
AU Mikhailov, S. N.; Padyukova, N. Sh.; Karpeiskii, M. Ya.; Kolobushkina, L. I.; Beigelman, L. N.
CS Inst. Mol. Biol.
LO Moscow 117984, USSR
SO Collect. Czech. Chem. Commun., 54(4), 1055-66
SC 33-9 (Carbohydrates)
DT J
CO CCCCAK
IS 0010-0765
PY 1989
LA Eng
OS CASREACT 112:36339
AN CA112(5):36339n
GI



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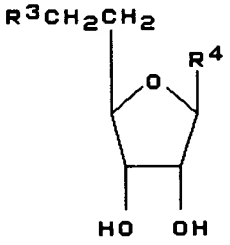


II

AB The conversion of hexofuranoses I [R1 = OCPh3, P(O)(OEt)2; R2 = H, PhCO] into ribohexofuranose nucleosides and phosphonate nucleotides II [R3 = OH, P(O)(OH)2; R4 = uracil residue, adenine residue] is reported.
IT 22415-88-9P 30685-57-5P 113808-29-0P 114071-55-5P 114071-57-7P 124572-49-2P 124572-50-5P 124572-51-6P 124572-52-7P 124572-53-8P
(prepn. of)

L5 ANSWER 10 OF 32 COPYRIGHT 1992 ACS
AN CA109(25):231447m
TI Synthesis of 4′-(hydroxymethyl)guanosine and a phosphonate analog of guanylic acid
AU Martin, John C.; Verheyden, Julien P. H.
CS Syntex Res.
LO Palo Alto, CA 94304, USA
SO Nucleosides Nucleotides, 7(3), 365-74
SC 33-9 (Carbohydrates)
SX 1, 10
DT J
CO NUNUD5
IS 0732-8311
PY 1988
LA Eng
OS CASREACT 109:231447
AN CA109(25):231447m
GI

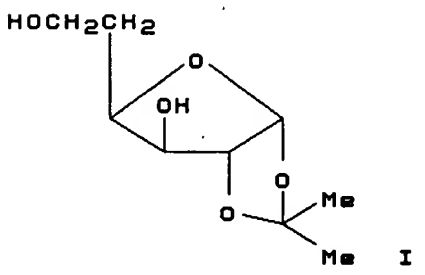
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The synthesis of 4′-(hydroxymethyl)guanosine (I) and the phosphonate analog II of guanylic acid proceed from a common intermediate, 2′,3′-O-isopropylidene-N2-(monomethoxytrityl)-guanosine-5′-aldehyde (III). I and II were found inactive when tested in vitro against herpes simplex virus types 1 and 2, parainfluenza 3, and respiratory syncytial virus.

IT 117544-95-3P
(prepn. and debenzylation of)

IT 85-32-5DP, Guanylic acid, phosphonate analog 117513-89-0P 117513-90-3P 117513-91-4P 117513-96-9P
(prepn. of)

L5 ANSWER 11 OF 32 COPYRIGHT 1992 ACS
AN CA108(21):187168z
TI A new scheme for the synthesis of 5′-nucleotide phosphonate analogs
AU Padyukova, N. Sh.; Karpeiskii, M. Ya.; Kolobushkina, L. I.; Mikhailov, S. N.
CS Inst. Mol. Biol.
LO Moscow 117984, USSR
SO Tetrahedron Lett., 28(31), 3623-6
SC 33-9 (Carbohydrates)
DT J
CO TELEAY
IS 0040-4039
PY 1987
LA Eng
OS CASREACT 108:187168
AN CA108(21):187168z
GI



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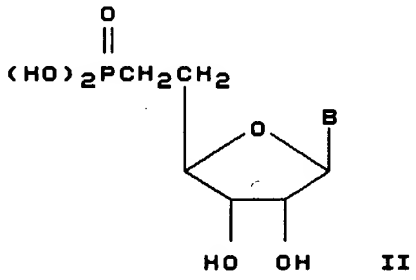


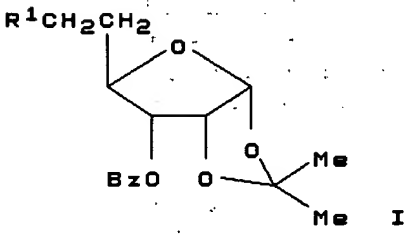
II

AB A convenient and general method is proposed for the synthesis of 5′-nucleotide phosphonate analogs starting from 5-deoxy-1,2-O-isopropylidene-.alpha.-D-xylo-hexofuranose (I). Nucleotide phosphonates II (B = uracilyl, adeninyl) were prepd. from I in several steps. Phosphonate-contg. sugar was prepd. by Arbuzov reaction and was then used for glycosylation.

IT 6490-42-2P 7307-92-8P 22257-15-4P 114071-57-7P
(prepn. of)

L5 ANSWER 12 OF 32 COPYRIGHT 1992 ACS
AN CA108(19):167857v
TI A new synthetic route to phosphonate analogs of 5′-nucleotides
AU Padyukova, N. Sh.; Karpeiskii, M. Ya.; Kolobushkina, L. I.; Mikhailov, S. N.
CS Inst. Mol. Biol.

LO Moscow, USSR
SO Bioorg. Khim., 13(5), 706-7
SC 33-9 (Carbohydrates)
DT J
CO BIKHD7
PY 1987
LA Russ
AN CA108(19):167857v
GI



AB Isosteric phosphonic acid analogs of 5′-nucleotides were prepd. from D-glucose which was converted via a series of reactions to 3-O-benzoyl-6-bromo-5,6-dideoxy-1,2-O-isopropylidene-.alpha.-D-ribo-hexofuranose (I). I underwent an Arbuzov reaction with (EtO)3P to give the phosphonate deriv., which was converted to the desired phosphonate analogs of 5′-nucleotides by acetolysis and coupling with trimethylsilyl derivs. of nucleic bases followed bydeblocking.
IT 7307-92-8P 22257-15-4P
(prepn. of)

L5 ANSWER 13 OF 32 COPYRIGHT 1992 ACS
AN CA107(21):193874x
TI Inhibition of phosphatidylinositol kinase in vascular smooth muscle membranes by adenosine and related compounds
AU Doctrow, Susan R.; Lowenstein, John M.
CS Grad. Dep. Biochem., Brandeis Univ.
LO Waltham, MA 02254, USA
SO Biochem. Pharmacol., 36(14), 2255-62
SC 7-3 (Enzymes)
DT J
CO BCPCA6
IS 0006-2952
PY 1987
LA Eng
AN CA107(21):193874x
AB Adenosine 5′-chloro-5′-deoxyadenosine inhibited the phosphorylation of phosphatidylinositol in membranes prepd. from aortic smooth muscle. The nucleosides did not affect the breakdown of phosphatidylinositol 4-phosphate. Under certain conditions, the membrane-bound phosphatidylinositol kinase phosphorylated exogenous phosphatidylinositol. The nucleosides inhibited the enzyme competitively with respect to Mg-ATP and noncompetitively with respect to phosphatidylinositol. Adenosine analogs modified in the ribose moiety were inhibitors with potencies comparable to that of adenosine, whereas adenine nucleotides and purine-modified adenosine analogs were much weaker inhibitors. D. gradient fractionation studies showed that phosphatidylinositol kinase is primarily assocd. with the sarcoplasmic reticulum. Since vascular smooth muscle contraction is assocd. with increased phosphatidylinositol turnover,

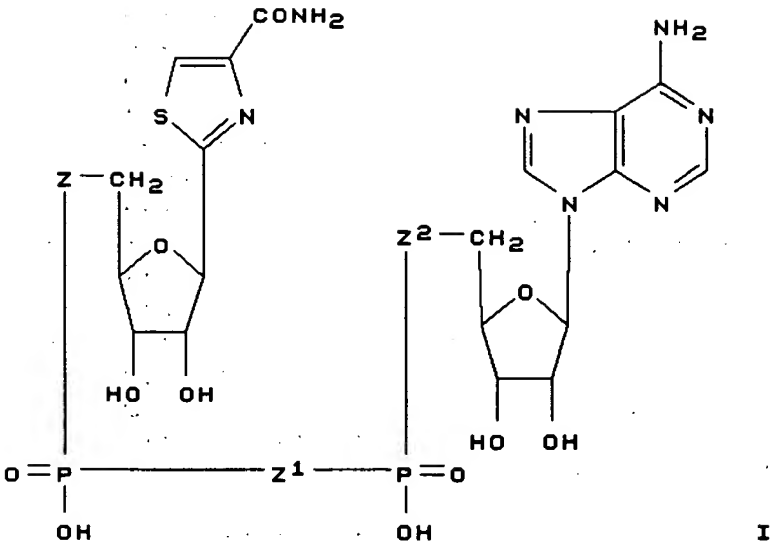
inhibition of phosphatidylinositol kinase by intracellular adenosine may be a factor involved in regulating vasodilation.
IT 58-61-7D, Adenosine, derivs. 58-64-0, 5′-ADP, biological studies 60-92-4, CAMP 61-19-8, 5′-AMP, biological studies 634-01-5 3768-14-7 4097-22-7, 2′,3′,-Dideoxyadenosine 19186-33-5, Aristeromycin 22257-15-4 34436-52-7 35920-39-9
(phosphatidylinositol kinase of vascular smooth muscle membranes inhibition by)

L5 ANSWER 14 OF 32 COPYRIGHT 1992 ACS
AN CA107(21):190370u
TI The structure-activity relationships of ectonucleotidases and of excitatory P2-purinoceptors: evidence that dephosphorylation of ATP analogs reduces pharmacological potency
AU Welford, Laurence A.; Cusack, Noel J.; Hourani, Susanna M. O.
CS King's Coll., Univ. London
LO London WC2R 2LS, UK
SO Eur. J. Pharmacol., 141(1), 123-30
SC 1-3 (Pharmacology)
DT J
CO EJPHAZ
IS 0014-2999
PY 1987
LA Eng
AN CA107(21):190370u
AB The dephosphorylation of adenine nucleotides and their analogs by ectonucleotidases on the guinea pig urinary bladder was studied using HPLC. The rate of dephosphorylation of each analog was compared with its pharmacol. potency at causing contraction. ATP, ADP, and AMP were rapidly dephosphorylated, and substitution on the purine ring did not affect the rate of breakdown. The ectonucleotidases showed stereoselectivity towards the ribose moiety and towards the polyphosphate chain. In general, methylene isosteres of the nucleotides, and analogs in which 1 of the O atoms on the terminal phosphate had been replaced, were resistant to degrdn. None of the analogs that were readily dephosphorylated was more potent than ATP, and most, but not all, of the analogs resistant to degrdn. were more potent than ATP, suggesting that although resistance to degrdn. does not in itself confer high potency, susceptibility to degrdn. does limit the potency of ATP and its degradable analogs.
IT 56-65-5, 5′-ATP, biological studies 56-65-5D, 5′-ATP, analogs 58-61-7, Adenosine, biological studies 58-64-0, ADP, biological studies 58-64-0D, ADP, analogs 61-19-8, 5′-AMP, biological studies 61-19-8D, 5′-AMP, analogs 63-39-8, UTP 65-47-4, CTP 73-24-5D, Adenine, nucleotides 86-01-1, GTP 146-77-0, 2-Chloroadenosine 2946-39-6, 8-Bromoadenosine 3080-29-3, L-Adenosine 4105-39-9, 2-Methyl-thioadenosine 7292-42-4 15214-89-8, AMPS 16506-88-0, 2-Chloro-ADP 21138-49-8 21466-01-3, 2-Chloro-AMP 22140-20-1, 2-Methylthio-AMP 22257-15-4 23567-96-6 23567-97-7 23589-16-4 23600-16-0, 8-Bromo-ADP 25612-73-1 34069-58-4 34983-48-7, 2-Methylthio-ADP 35094-45-2 35094-46-3 37515-63-2 43170-89-4, 2-Methylthio-ATP 49564-60-5, 2-Chloro-ATP 52830-41-8 58976-48-0 58976-49-1 59261-35-7 59261-36-8 59286-20-3 59331-71-4 72041-44-2 72635-67-7, 2-Chloro-L-adenosine 72635-68-8 72635-69-9 87147-73-7 87147-74-8 96156-15-9 105701-90-4 105701-91-5 105701-92-6 105740-45-2 105740-46-3 105740-47-4 105815-86-9 107284-95-7
(bladder contraction by, structure in relation to)

L5 ANSWER 15 OF 32 COPYRIGHT 1992 ACS
AN CA106(3):12328h

TI ATP analogs and the guinea pig tenia coli: a comparison of the structure-activity relationships of ectonucleotidases with those of the P2-purinoceptor
AU Welford, Laurence A.; Cusack, Noel J.; Hourani, Susanna M. O.
CS King's Coll., Univ. London
LO London WC2R 2LS, UK
SO Eur. J. Pharmacol., 129(3), 217-24
SC 1-3 (Pharmacology)
SX 13
DT J
CO EJPHAZ
IS 0014-2999
PY 1986
LA Eng
AN CA106(3):12328h
AB The dephosphorylation of adenine nucleotides and their analogs by ectonucleotidase [9027-73-0] in the guinea pig tenia coli was studied using HPLC. The rate of dephosphorylation of each analog was compared with its pharmacol. potency relative to ATP [56-65-5]. ATP, ADP [58-64-0] and AMP [61-19-8] were rapidly dephosphorylated, and substitution on the purine ring had no effect upon the rate of breakdown. The ectonucleotidases showed stereoselectivity towards the ribose, the unnatural L-enantiomers of nucleotides being dephosphorylated more slowly. Analogs in which one of the O atoms on the terminal phosphate had been replaced were resistant to degrdn. Phosphorothioate analogs in which a sulfur was attached to the penultimate phosphorus were degraded stereoselectively. Methylene isosteres of ATP and ADP resisted degrdn., except for homo-ATP [72041-44-2] which was dephosphorylated at the same rate as ATP. Overall, no correlation was found between the potency of an analog and its rate of degrdn.
IT 56-65-5D, ATP, analogs 3080-29-3, L-Adenosine 21138-49-8, L-AMP 22257-15-4 23589-16-4, N6-Phenyladenosine 34069-58-4, L-ADP 37515-63-2 51777-22-1, Adenosine 5'-O-(1-thiodiphosphate) 52830-41-8 58175-53-4, L-ATP 58976-48-0 58976-49-1 59261-35-7 59261-36-8 59286-20-3 59331-71-4 72635-67-7, 2-Chloro-L-adenosine 72635-68-8 72635-69-9 80257-10-9 87147-73-7 87147-74-8 96156-15-9 105740-45-2 105815-86-9 107284-95-7
(metab. of, by ectonucleotidase of tenia coli, P2-purinergic activity in relation to)

L5 ANSWER 16 OF 32 COPYRIGHT 1992 ACS
AN CA105(11):97866j
TI Thiazole-4-carboxamide adenine dinucleotide (TAD). Analogs stable to phosphodiesterase hydrolysis
AU Marquez, Victor E.; Tseng, Christopher K. H.; Gebeyehu, Gulilat; Cooney, David A.; Ahluwalia, Gurpreet S.; Kelley, James A.; Dalal, Maha; Fuller, Richard W.; Wilson, Yvonne A.; Johns, David G.
CS Lab. Pharmacol. Exp. Ther., Natl. Cancer Inst.
LO Bethesda, MD 20205, USA
SO J. Med. Chem., 29(9), 1726-31
SC 33-9 (Carbohydrates)
SX 1
DT J
CO JMCMAR
IS 0022-2623
PY 1986
LA Eng
OS CASREACT 105:97866; CJACS
AN CA105(11):97866j
GI



I

AB Thiazole-4-carboxamide adenine dinucleotide (I; Z = Z1 = Z2 = O; TAD), the active metabolite of the oncolytic C-nucleotide tiazofurin (TR), is susceptible to phosphodiesteratic breakdown by a unique phosphodiesterase present at high levels in TR-resistant tumors. Since accumulation of TAD, as regulated by its synthetic and degradative enzymes, appears to be an important determinant for sensitivity to the drug, a series of hydrolytically resistant phosphonate analogs of TAD were synthesized with the intent of producing more stable compds. with an ability to inhibit IMP dehydrogenase equiv. to TAD itself. Isosteric phosphonic acid analogs of TR and adenosine nucleotides were coupled with activated forms of AMP and TR monophosphate to give dinucleotides I (Z = CH2, Z1 = Z2 = O; Z = Z1 = O, Z2 = CH2). Coupling of protected adenosine 5′-(.alpha.,.beta.-methylene)diphosphate with isopropylidene-TR in the presence of DCC afforded I (Z = Z2 = O, Z1 = CH2) (II) after deprotection. These compds. are more resistant than TAD toward hydrolysis and still retain potent activity against IMP dehydrogenase in vitro. .beta.-Methylene-TAD (I), the most stable of the TAD phosphonate analogs, produced a depletion of guanine nucleotide pools in an exptl. induced TR-resistant P388 tumor variant that was superior to that obtained with TR in the corresponding sensitive line.

IT 22257-15-4
(coupling of, with tiazofurin phosphate deriv.)

L5 ANSWER 17 OF 32 COPYRIGHT 1992 ACS
AN CA102(21):181349p
TI 5′-Nucleotidase from rat heart membranes. Inhibition by adenine nucleotides and related compounds
AU Naito, Yoshitsugu; Lowenstein, John M.
CS Grad. Dep. Biochem., Brandeis Univ.
LO Waltham, MA 02254, USA
SO Biochem. J., 226(3), 645-51
SC 7-3 (Enzymes)
DT J
CO BIJOAK
IS 0306-3275

PY 1985
LA Eng
AN CA102(21):181349p
AB ADP and ATP and their analogs were evaluated as inhibitors of 5′-nucleotidase purified from heart plasma membrane. ADP analogs were more powerful inhibitors than the corresponding ATP analogs. The most powerful inhibitor found was adenosine 5′-[.alpha..beta.-methylene]diphosphate (AOPCP) for which the enzyme showed a Ki of 5 nM at pH 7.2. Measurements of pKi values for ADP and AOPCP as a function of pH indicated that the major inhibitory species of both nucleotides was the dianion. In the physiol. range of pH values, AOPCP was a more powerful inhibitor than ADP principally because a higher percentage of AOPCP exists in the dianion form. The methylenephosphonate analog of AMP (ACP), although not a substrate, was a moderately effective inhibitor. The corresponding analogs of ADP (ACPOP) and ATP (ACPOPOP) were as good inhibitors as ADP and ATP, resp. The thiophosphate analogs of ADP all inhibited 5′-nucleotidase, although not as powerfully as ADP, the most effective of these analogs being adenosine 5′-O-(1-thiodiphosphate) diastereoisomer B [ADP[.alpha.S](B)]. Other nucleotides inhibited the enzyme, but none was as effective as AOPCP. Inorg. tripolyphosphate and methylenediphosphonate were better inhibitors of the enzyme than was inorg. pyrophosphate. Inorg. thiophosphate was a better inhibitor than was orthophosphate. Hill plots of the ADP and AOPCP inhibition yielded slopes close to 1; Hill plots of the ATP inhibition yielded slopes of .apprx.0.6. MgADP- was not an inhibitor, and MgATP2- was at best a very weak inhibitor of the enzyme.
IT 56-65-5, biological studies 58-61-7, biological studies 58-64-0, biological studies 1984-15-2 3469-78-1 3768-14-7 7292-42-4 14000-31-8 14127-68-5 14265-44-2, biological studies 15106-26-0 15181-41-6 22257-15-4 35094-45-2 38806-39-2 59286-20-3 59331-71-4 72041-44-2 96156-15-9
(5′-nucleotidase of heart inhibition by, kinetics of)

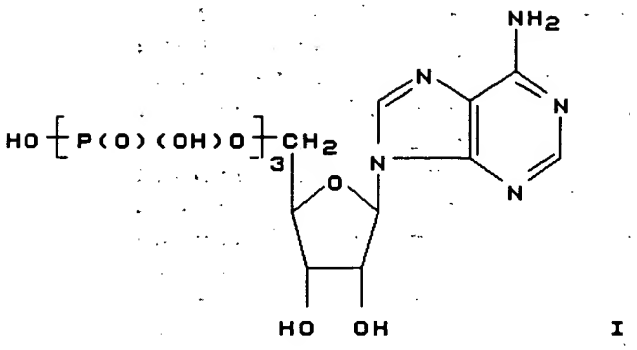
L5 ANSWER 18 OF 32 COPYRIGHT 1992 ACS
AN CA98(17):137998z
TI Inhibitory purinergic receptors in visceral smooth muscle
AU Satchell, David G.; Maguire, M. Helen
CS Dep. Zool., Univ. Melbourne
LO Parkville, Australia
SO Physiol. Pharmacol. Adenosine Deriv., [Proc. Meet.], Meeting Date 1981, 85-95. Edited by: Daly, John W. Raven: New York, N. Y.
SC 2-8 (Mammalian Hormones)
DT C
CO 49DRAD
PY 1983
LA Eng
AN CA98(17):137998z
AB ATP [56-65-5] And ADP [58-64-0] showed similar dose-response curves in inducing relaxation of tenia coil prepns., as did AMP [61-19-8] and adenosine [58-61-7]; however, the latter compds. were less effective than ATP or ADP. All of these compds. were similar in their relaxation of tracheal strips. This suggests that the tenia coli contains 2 types of purinergic receptors and that the trachea has a single type. Structure-activity relations for a no. of adenosine derivs. were also discussed.
IT 56-65-5, biological studies 58-61-7, biological studies 58-64-0, biological studies 61-19-8, biological studies 958-09-8 1927-31-7 2946-39-6 3714-60-1 4105-39-9 5536-17-4 22257-15-4 23567-97-7 43170-89-4 72041-44-2
(smooth muscle relaxation by, purinergic receptors in relation

to)

L5 ANSWER 19 OF 32 COPYRIGHT 1992 ACS
AN CA97(1):2705k
TI Species- or isozyme-specific enzyme inhibitors. 7. Selective effects in inhibitions of rat adenylate kinase isozymes by adenosine 5′-phosphate derivatives
AU Hai, Ton T.; Picker, Donald; Abo, Masanobu; Hampton, Alexander
CS Fox Chase Cancer Cent., Inst. Cancer Res.
LO Philadelphia, PA 19111, USA
SO J. Med. Chem., 25(7), 806-12
SC 7-3 (Enzymes)
DT J
CO JMCMAR
IS 0022-2623
PY 1982
LA Eng
OS CJACS
AN CA97(1):2705k
AB Monosubstituted derivs. of AMP with substituents of 1-3 atoms or group replacements at any of 11 positions were synthesized and examd. as substrates and inhibitors of the rat muscle adenylate kinase isoenzyme (AK-M) and the rat AK II and III isoenzymes predominant in poorly differentiated hepatoma tissue and normal liver tissue, resp. Inhibition indexes of the compds. were expressed as Km(AMP)/Ki for competitive inhibition or as Km(AMP)/Km when only Km was available. Substituents at N(1), N6, or C(8) or on the ionizable phosphate O atom reduced inhibition below measurable levels; 2′-deoxy-AMP and adenosine 5′-sulfate had identical inhibition indexes with all 3 isoenzymes; compds. with substituents at C(2), O(2′), O(3′), C(4′), C(5′), or O(5′) had higher inhibition indexes with AK-M than with AK II or III, and the same or similar indexes for AK II and III. The most effective and(or) selective inhibitors were 2-NHMe-AMP (index with AK-M, 0.2; index ratio, AK-M/AK III, 9.1), 2′-O-Me-AMP (index with AK-M, 0.14; index ratio, AK-M/AK III, 8.2), 2′,3′-O-CMe2-AMP (index with AK-M, 0.25; index ratio, AK-M/AK II, 6.6), 4′-allyl-AMP (index with AK-M, 0.97; index ratio, AK-M/AK III, 8.1), and 5′(S)-Et-AMP (index with AK-M, 0.64; index ratio, AK-M/AK II, 11.2). The study provided addnl. evidence that the attachment of simple substituents to various atoms in turn of a substrate is a potentially useful approach in early stages of the attempted design of isoenzyme-selective inhibitors.
IT 2922-74-9 13039-54-8 34212-86-7 81921-27-9 81921-28-0 81921-29-1 81921-30-4 81921-33-7 81969-05-3 (reaction of, with adenylate kinase isoenzymes, structure in relation to)

L5 ANSWER 20 OF 32 COPYRIGHT 1992 ACS
AN CA92(15):122602t
TI Specificity of adenine nucleotide receptor sites: inhibition of the guinea pig taenia coli by adenine nucleotide analogs
AU Maguire, M. Helen; Satchell, D. G.
CS Ralph L. Smith Ment. Retard. Res. Cent., Univ. Kansas
LO Kansas City, KS 66103, USA
SO Physiol. Regul. Funct. Adenosine Adenine Nucleotides, [Proc. Conf.], Meeting Date 1978, 33-43. Edited by: Baer, Hans P.; Drummond, George I. Raven: New York, N. Y.
SC 3-5 (Biochemical Interactions)
DT C
CO 41FPAT
PY 1979
LA Eng

AN CA92(15):122602t
GI



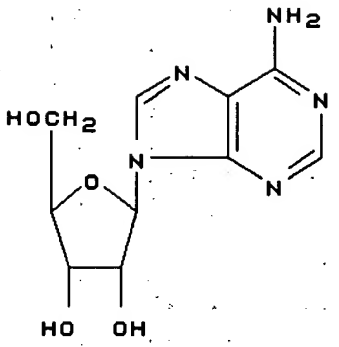
I

AB Alterations in the purine ring, sugar moiety, and triphosphate chain of ATP [56-65-5] modified, but did not abolish, the inhibitory activity on contractions in guinea pig tenia coli prepns. Contraction-inhibiting activity was substantially decreased with 8-substitution of the purine ring, whereas only modest decreases in activity were obsd. with epimerization of the 2′-hydroxyl or with alteration of the triphosphate function. The agonistic activities of 2-chloro-ATP [49564-60-5], 2-methylthio-ADP [34983-48-7], 2-methylthio-ATP [43170-89-4], and 6′-deoxyhomoadenosine 6′-phosphonyldiphosphate [72041-44-2] were 3.1-, 30-, 50-, and 70.8-fold higher than that of I, resp. 5-Methylthio- and 2-chloro-substituted derivs. of AMP and adenosine also caused inhibition of contraction, but these derivs. took 3 times as long as I to reach max. relaxation. Different receptor populations may be involved in the contraction inhibition, 1 receptor for I and ADP [58-64-0] and another receptor for adenosine [58-61-7] and AMP [61-19-8].

IT 56-65-5, biological studies 58-61-7, biological studies 58-64-0, biological studies 61-19-8, biological studies 73-24-5D, nucleotides 146-77-0 1062-98-2 3469-78-1 3768-14-7 4105-39-9 7292-42-4 16506-88-0 21466-01-3 22140-20-1 22257-15-4 34983-48-7 35057-44-4 43170-89-4 49564-60-5 50676-82-9 50880-71-2 72041-44-2 (intestine relaxation by)

L5 ANSWER 21 OF 32 COPYRIGHT 1992 ACS
AN CA91(25):205079h
TI Effects of adenosine and adenine nucleotides in synaptic transmission in the cerebral cortex
AU Phillis, J. W.; Edstrom, J. P.; Kostopoulos, G. K.; Kirkpatrick, J. R.
CS Coll. Med., Univ. Saskatchewan
LO Saskatoon, SK, Can.
SO Can. J. Physiol. Pharmacol., 57(11), 1289-312
SC 3-5 (Biochemical Interactions)
DT J
CO CJPPA3
IS 0008-4212
PY 1979
LA Eng
AN CA91(25):205079h

GI



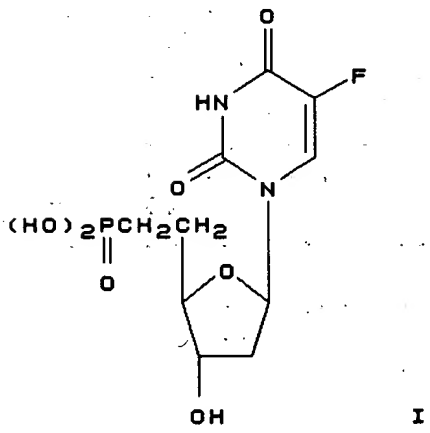
I

AB Adenosine (I) [58-61-7] and the adenine nucleotides had a potent depressant action on cerebral cortical neurons, including identified corticospinal cells. Other purine and pyrimidine nucleotides were either weakly depressant or largely inactive as depressants.. The 5′-triphosphates and to a lesser extent the 5′-diphosphates of all the purine and pyrimidines tested had excitant actions on cortical neurons. I transport blockers and deaminase inhibitors depressed the firing of cortical neurons and potentiated the depressant actions of I and the adenine nucleotides. Methylxanthines antagonized the depressant effects of I and the adenine nucleotides and enhanced the spontaneous firing rate of cerebral cortical neurons and suppressed spontaneous and evoked excitatory postsynaptic potentials in the absence of any pronounced alterations in membrane resistance or of the threshold for action potential generation. I may depress spontaneous and evoked activity by inhibiting the release of transmitter from presynaptic nerve terminals. Furthermore, the depressant effects of potentiators and excitant effects of antagonists of I on neuronal firing are consistent with the hypothesis that cortical neurons are subject to control by endogenously released purines.

IT 50-89-5, biological studies 53-59-8 56-65-5, biological studies 58-32-2 58-55-9, biological studies 58-61-7, biological studies 58-63-9 58-64-0, biological studies 58-96-8 58-97-9, biological studies 60-92-4 61-19-8, biological studies 61-25-6 63-37-6 63-39-8 65-47-4 68-94-0 69-33-0 69-89-6 73-03-0 73-24-5, biological studies 84-21-9 84-52-6 84-53-7 85-32-5 85-61-0, biological studies 85-94-9 86-01-1 118-00-3, biological studies 130-49-4 131-83-9 131-99-7 132-06-9 146-17-8 146-76-9 146-77-0 146-78-1 146-80-5 146-91-8 146-92-9 365-07-1 365-08-2 523-98-8 524-69-6 550-33-4 634-01-5 653-63-4 890-38-0 958-09-8 1053-73-2 1062-98-2 1333-74-0, biological studies 1818-71-9 2096-10-8 2304-12-3 2596-55-6 2946-39-6 3416-26-0 3469-78-1 3768-14-7 3805-37-6 4754-39-6 6253-56-1 7292-42-4 15731-72-3 16177-21-2 22257-15-4 23589-16-4 28822-58-4 32476-54-3 37151-17-0 41094-07-9 41708-91-2 53910-25-1 56583-49-4 72007-82-0
(synaptic neurotransmission response to)

L5 ANSWER 22 OF 32 COPYRIGHT 1992 ACS
AN CA90(13):97373t
TI Phosphonate analog of 2′-deoxy-5-fluorouridylic acid
AU Montgomery, John A.; Thomas, H. Jeanette
CS Sch. Med., Tufts Univ.

LO Boston, Mass., USA
SO J. Med. Chem., 22(1), 109-11
SC 1-4 (Pharmacodynamics)
SX 33
DT J
CO JMCMAR
IS 0022-2623
PY 1979
LA Eng
AN CA90(13):97373t
GI

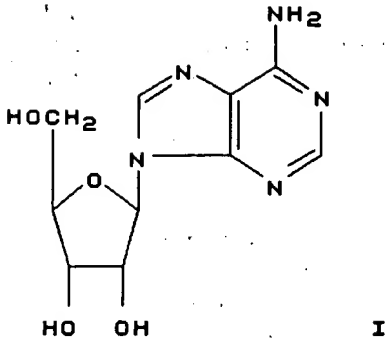


I

AB Ba 1-(2′,5′,6′-trideoxy-.beta.-D-ribohexofuranosyl)-5-fluorouracil-6′-phosphonate (I Ba) [69124-08-9] was prepd. by the oxidn. of 3′-O-acetyl-2′-deoxy-5-fluorouridine [2059-38-3] to the aldehyde, reaction of the aldehyde with diphenyl(triphenylphosphoranylidene)methylphosphonate [22400-41-5], to give the olefin, and redn. of the olefin to a satd. compd. followed by treatment with 3N NaOH. I inhibited thymidylate synthetase [9031-61-2] from Lactobacillus casei, Escherichia coli and Coliphage T2, and was cytotoxic to H. Ep-2 cells in culture.

IT 69124-08-9P
(prepn. of and thymidylate synthetase inhibition by)

L5 ANSWER 23 OF 32 COPYRIGHT 1992 ACS
AN CA85(23):171551q
TI Adenosine inhibition of isolated rabbit ileum and antagonism by theophylline
AU Ally, Ariff I.; Nakatsu, Kanji
CS Fac. Med., Queen's Univ.
LO Kingston, Ont., Can.
SO J. Pharmacol. Exp. Ther., 199(1), 208-15
SC 1-3 (Pharmacodynamics)
SX 13
DT J
CO JPETAB
PY 1976
LA Eng
AN CA85(23):171551q
GI



I

AB The spontaneously contracting isolated rabbit ileum was used to study adenosine (I) [58-61-7]-stimulated receptors. The inhibitory effects of I were not reduced by pretreating the rabbits with either reserpine or 6-hydroxydopamine which were used to eliminate adrenergic function. Similarly the addn. of tetrodotoxin to the muscle bath had no effect on the ability of adenosine to produce its inhibitory response. Of the compds. tested for agonistic activity, I and ATP [56-65-5] were the most potent (ED50 .simeq. 6 .times. 10-7 M). The inhibition by I was antagonized by both theophylline [58-55-9] and caffeine [58-08-2] in a surmountable manner. Theophylline analogs with charged substituents in position 7 were without antagonist activity. The results suggest that receptors for I or adenine nucleotides are located on the smooth muscle cells of rabbit ileum, receptor stimulation requires an intact I moiety and methylxanthines exert their antagonistic effects by acting as competive angagonists.

IT 56-65-5, biological studies 58-61-7, biological studies 61-19-8, biological studies 63-37-6 73-03-0 73-24-5, biological studies 85-32-5 131-99-7 362-74-3 365-07-1 550-33-4 653-63-4 1867-73-8 14675-48-0 22257-15-4
(intestine contraction inhibition by, adenosine receptors in relation to)

L5 ANSWER 24 OF 32 COPYRIGHT 1992 ACS
AN CA85(3):16175b
TI Evidence for the conformation about the C(5′)-O(5′) bond of AMP complexed to AMP kinase: substrate properties of a vinyl phosphonate analog of AMP
AU Hampton, Alexander; Kappler, Francis; Perini, Florian
CS Inst. Cancer Res., Fox Chase Cancer Cent.
LO Philadelphia, Pa., USA
SO Bioorg. Chem., 5(1), 31-5
SC 7-3 (Enzymes)
DT J
CO BOCMBM
PY 1976
LA Eng
AN CA85(3):16175b
AB A vinyl phosphonate analog of AMP was synthesized in which the CH2-O-P system of AMP is replaced by CH:CH-P. The Vmax values of this analog relative to AMP were 0.7% with rabbit muscle AMP aminohydrolase, 13.4% with rabbit muscle AMP kinase, and 6.6% with pig muscle AMP kinase. The vinyl analog of ADP produced by the kinase was a substrate of rabbit muscle pyruvate kinase. These results, together with substrate specificity properties at the AMP sites of the enzymes indicate that the C(4′)-C(5′)-O(5′)-P system of

AMP is of trans character during conversion of AMP to ADP by pig or rabbit AMP kinase.
IT 22257-15-4 59652-80-1
(AMP kinase and AMP aminohydrolase specificity for)

L5 ANSWER 25 OF 32 COPYRIGHT 1992 ACS
AN CA84(13):84882j
TI Inhibitory effects of adenine nucleotide analogs on the isolated guinea pig taenia coli
AU Satchell, D. G.; Maguire, M. Helen
CS Dep. Zool., Univ. Melbourne
LO Parkville, Aust.
SO J. Pharmacol. Exp. Ther., 195(3), 540-8
SC 3-5 (Biochemical Interactions)
DT J
CO JPETAB
PY 1975
LA Eng
AN CA84(13):84882j
AB The inhibitory actions of ADP [58-64-0], AMP [61-19-8],adenosine [58-61-7], and 16 adenine nucleotide and nucleoside analogs on the isolated guinea pig taenia coli prepn. were compared with those of ATP [56-65-5]. Responses were quantitated as magnitude of maximal relaxation, time taken to reach maximal relaxation, and activity relative to that of ATP. Inhibitory responses induced by 2-chloroadenosine di- [16506-88-0] and triphosphate [49564-60-5] and 2-methylthioadenosine di- [34983-48-7] and triphosphate [43170-89-4] resembled those elicited by ADP and ATP, but the 2-substituted analogs were markedly more potent. AMP and adenosine were less active than ATP; their activities were enhanced by 2-chloro substitution but not by 2-methylthio substitution. 2-Methylthio-AMP [22140-20-1] and 2-methylthioadenosine [4105-39-9] were the only analogs which did not elicit maximal relaxation of the taenia coli. 6′-Deoxyhomoadenosine 6′-phosphonic acid [22257-15-4] was inactive. Adenine nucleotide analogs in which the polyphosphate moiety was modified had steeper log dose-response curves than ATP and induced greater maximal responses than ATP. Analogs in which the polyphosphate .alpha. .beta.-anhydride O was replaced by methylene took .ltoreq.5 times longer than ATP to cause maximal relaxation. Other analogs with modified or unmodified polyphosphate side chains caused rapid relaxation of the taenia coli. There was no apparent correlation between relative activity and time to reach maximal response. Apparently, di- or triphosphate groupings are of prime importance in binding adenine nucleotides to the putative smooth muscle receptor which mediates their inhibitory responses, and hydrolysis of the terminal phosphates of adenosine 5′-polyphosphates may not be a requirement for inhibitory activity. Reasons for the distinctive inhibitory actions of the phosphate-modified adenine nucleotide analogs are discussed.
IT 56-65-5, biological studies 58-61-7, biological studies 58-64-0, biological studies 61-19-8, biological studies 146-77-0 3469-78-1 3768-14-7 4105-39-9 16506-88-0 21466-01-3 22140-20-1 22257-15-4 34983-48-7 43170-89-4 49564-60-5 58337-42-1 58337-43-2 58337-45-4 58337-46-5 58337-47-6
(intestine relaxation by)

L5 ANSWER 26 OF 32 COPYRIGHT 1992 ACS
AN CA81(19):114436z
TI Synthesis and enzymic activity of 1,2,4-triazole-3-carboxamide 6′-deoxyhomoribonucleoside-6′-phosphonic acid and related compounds
AU Fuertes, Mercedes; Witkowski, Joseph T.; Streeter, David G.; Robins,

Roland K.
CS Nucleic Acid Res. Inst., ICN Pharm., Inc.
LO Irvine, Calif., USA
SO J. Med. Chem., 17(6), 642-5
SC 1-4 (Pharmacodynamics)
SX 33
DT J
CO JMCMAR
PY 1974
LA Eng
AN CA81(19):114436z
AB Of 4 title compds., prepd. from 1-(2,3-O-isopropylidene-.beta.-D-ribo-pento-1,5-dialdo-1,4-furanosyl)-1,2,4-triazole-3-carboxamide [52663-92-0] by the Wittig reaction followed by hydrogenation and deacetalization, 1-(5,6-dideoxy-.beta.-D-ribo-hexofuranosyl-6-phosphonic acid)-1,2,4-triazole-3-carboxamide (I) [52663-96-4] was the only inhibitor of inosine 5′-phosphate dehydrogenase [9028-93-7]. None of the compds showed antiviral activity in tests against type 3 adeno, type 1 herpes simplex, type 13 rhino, and type 3 parainfluenza viruses.
IT 52663-96-4P 52663-98-6P 52663-99-7P 52664-00-3P
(prepn. and biol. activity of)

L5 ANSWER 27 OF 32 COPYRIGHT 1992 ACS
AN CA75(21):130083p
TI Phosphorylated phosphonium ylids
CS Syntex Corp.
SO Brit., 22 pp.
PI GB 1243213 18 Aug 1971
PRAI US 18 Jul 1967 - 29 Feb 1968
IC C07F
SC 33 (Carbohydrates)
DT P
CO BRXXAA
PY 1971
LA Eng
AN CA75(21):130083p
AB The title compds. (I) are prepd. by condensing a monosubstituted phosphonium ylide with a phosphoryl halide in an inert solvent. I are converted into nucleoside 6′-phosphonates. Thus, 1.6M BuLi in hexane was added to methyltriphenylphosphonium bromide in ether at 20.degree.. After 0.5 hr, diphenyl phosphorochloridate in ether was slowly added and the product acidified and neutralized to give di-Ph triphenyl-phosphoranylidenemethylphosphonate (II). 2,3′-O-Anisylideneuridine-5′-carboxaldehyde was warmed 16 hr with II in THF to give di-Ph [1-(2,3-O-anisylidene-5,6-dideoxy-.beta.-D-ribo-hex-5-enofuranosyl)uracil] 6′-phosphonate.
IT 7307-92-8P 22257-13-2P 31080-06-5P 31080-07-6P
31199-53-8P 34212-86-7P 34213-68-8P 34213-70-2P
34213-71-3P 34295-88-0P 34393-60-7P 34393-67-4P
(prepn. of)

L5 ANSWER 28 OF 32 COPYRIGHT 1992 ACS
AN CA75(19):118548m
TI Nucleoside 6′-phosphonic acids and the corresponding phosphonates
CS Syntex Corp.
SO Brit., 10 pp. Division of Brit. 1,243,213.
PI GB 1243214 18 Aug 1971
PRAI US 18 Jul 1967 - 29 Feb 1968
IC C07F
SC 33 (Carbohydrates)

DT P
CO BRXXAA
PY 1971
LA Eng
AN CA75(19):118548m
AB Nucleoside 5′-aldehyde are converted into nucleoside 6′-phosphonic acids by the treatment of the aldehydes with phosphorylated phosphonium ylides. Thus, 2′,3-O-anisylideneuridine-5-aldehyde and Ph3P:CHP(O)(OPh)2 are kept 16 hr at 37.degree. in THF to give di-Ph [1-(2,3-O-anisylidene-5,6-dideoxy-.beta.-D-ribo-hex-5-enefuranosyl)uracil]-6′ -phosphonate.
IT 7307-92-8P 22257-13-2P 22400-41-5P 31080-06-5P
31080-07-6P 34204-53-0P 34212-85-6P 34212-86-7P
34213-65-5P 34213-66-6P 34213-68-8P 34213-70-2P 34213-71-3P
34295-88-0P 34295-89-1P
(prepn. of)

L5 ANSWER 29 OF 32 COPYRIGHT 1992 ACS
AN CA74(11):54150v
TI Physiologically active nucleoside phosphonates and phosphonic acids
AU Jones, Gordon Henry; Moffatt, John G.
CS Syntex Corp.
SO Ger. Offen., 74 pp.
PI DE 2009834 17 Sep 1970
PRAI US 10 Mar 1969
IC C07D; A61K
SC 33 (Carbohydrates)
DT P
CO GWXXBX
PY 1970
LA Ger
AN CA74(11):54150v
AB Phosphonates and phosphonic acids of .beta.-D-ribo-, xylo-, and -arabinofuranosyl-pyrimidines and purines are prepd. Examples are given for only ribofuranosyluracil derivs. in this abstr. CLCH2P(O)(OPh)2 was treated with Bu3P followed by aq. NaOH to give Bu3P:CHP(O)(OPh)2 (I). II was treated with Me2C(OMe)2 and (p-O2NC6H4)2-HPO4 to give III which was treated with N,N′-dicyclohexyl-carbodiimide-Me2SO-pyridine-F3CCO2H followed by I to give cis- and trans-IV. Catalytic hydrogenation (Pd/BaSO4) of IV gave V, while VI gave VII. V was heated with 80% HOAc to give VIII. Treatment of V with aq. LiOH gave IX which was incubated with Crotalus adamanteus (snake) esterase in tris(hydroxymethyl)aminomethane buffer to give VII. X was brominated with Br/CCl4 to give XI which was treated with MeNH2 to give XII. Di-Na salt of X was successively treated with Br-H2O, pyridine, and aq. Ba(OAc)2 to give di-Ba salt of XIII.
IT 362-43-6P 7307-92-8P 22257-13-2P 22257-15-4P
27999-65-1P 31079-96-6P 31079-97-7P 31079-98-8P 31080-00-9P
31080-01-0P 31080-02-1P 31080-03-2P 31080-04-3P 31080-05-4P
31080-06-5P 31080-07-6P 31080-08-7P 31080-09-8P 31080-11-2P
31080-13-4P 31087-98-6P 31087-99-7P
31198-98-8P 31199-53-8P 33072-52-5P
(prepn. of)

L5 ANSWER 30 OF 32 COPYRIGHT 1992 ACS
AN CA74(7):31940p
TI Didealkylation of phosphonate esters
AU Moffatt, John G.; Jones, Gordon H.
CS Syntex Corp.
SO U.S., 8 pp.
PI US 3524846 18 Aug 1970

AI US 2 Jun 1967
IC C07F
NCL 260211500
SC 33 (Carbohydrates)
DT P
CO USXXAM
PY 1970
LA Eng
AN CA74(7):31940p
AB Sensitive phosphonate esters, such as those of nucleosides, such as uridines, lipids, steroids, and sugars were didealkylated under mild, neutral conditions by heating tham at 140-50.degree. with metal iodides or bromides, such as NaI, in aprotic solvents, such as DMF or AcNMe2, for 15-36 hr. Thus, a mixt. of 3.5 g diethyl 2-hexadecycloxy-3-octadecyloxypropylphosphonate and 3 g NaI in 20 ml DMF was heated at 150.degree. for 20 hr to yield 2-hexadecyloxy-3-octadecyloxypropyl-1-phosphonic acid.
IT 688-64-2P 4933-77-1P 7533-93-9P 15106-36-2P
22257-15-4P 30685-49-5P 30685-50-8P 30685-51-9P
30685-52-0P 30685-53-1P 30685-55-3P 30685-56-4P 30685-57-5P
30685-58-6P 30685-60-0P 30685-61-1P 30685-62-2P 30685-63-3P
30685-64-4P 30685-65-5P 30784-78-2P 30784-79-3P 30784-80-6P
30784-81-7P 30784-82-8P 30784-83-9P 30784-85-1P 30784-86-2P
30784-87-3P 30784-88-4P 30784-89-5P 30784-91-9P 30784-92-0P
30902-94-4P 31675-01-1P 33192-71-1P
(prepn. of)

L5 ANSWER 31 OF 32 COPYRIGHT 1992 ACS
AN CA73(1):437e
TI Specific binding to adenylosuccinate synthetase of analogs of inosinic acid with nitrogen, sulfur, and carbon substituted for phosphate oxygens
AU Hampton, Alexander; Chu, Samuel Y.
CS Dep. Biochem., Univ. Alberta
LO Edmonton, Alberta, Can.
SO Biochim. Biophys. Acta, 198(3), 594-600
SC 3 (Enzymes)
DT J
CO BBACAQ
PY 1970
LA Eng
AN CA73(1):437e
AB Binding of the phosphate moiety of IMP to adenylosuccinate synthetase (EC 6.3.4.4) of Escherichia coli was investigated with the aid of analogs of IMP in which one phosphate oxygen of IMP was replaced by another atom. Inosine 5′-phosphorothiolate, 5′-mercapto-5′ - deoxyinosine 5′ - S - phosphate,5′ - amino - 5′ - deoxyinosine 5′-N-phosphate, and 6′-deoxyhomoinosine 6′-phosphonic acid substituted for IMP as substrates of the synthetase; in the presence of satg. levels of GTP and aspartate their Vmax values relative to IMP (Vmax = 1.00 were 0.024, 0.066, 0.0023, and 0.035, resp. The above 4 analogs and also AMP and 6′-deoxyhomoadenosine 6′-phosphonic acid were competitive inhibitors of the synthetase with respect to IMP with enzyme-inhibitor dissocn. consts. of 140, 70, 320, 490, 32, and 280 .mu.M, resp. The dissocn. const. of IMP was estd from these data to be approx. 50 .mu.M. The enzyme-substrate dissocn. const. of 5′-mercapto-5′-deoxyinosine 5′-S-phosphate together with data on its secondary phosphoryl pKa and the relative tendency of O and S to form H bonds was taken to indicate that IMP probably binds to the synthetase preferentially as its phosphodianion and that the O at C-5′ of IMP did not make a major contribution to IMP binding. It was suggested that steric

properties in the region of the phosphate group of IMP may exert a profound influence on spatial relations between substrates and the active site.
IT 21914-75-0 21959-63-7 21959-64-8 22257-15-4
25203-85-4
(reaction of, with adenylosuccinate synthetase, kinetics of)

L5 ANSWER 32 OF 32 COPYRIGHT 1992 ACS
AN CA70(1):4503j
TI The synthesis of 6′-deoxyhomonucleoside 6′-phosphonic acids
AU Jones, G. H.; Moffatt, J. G.
CS Inst. of Mol. Biol., Syntex Res.
LO Palo Alto, Calif., USA
SO J. Amer. Chem. Soc., 90(19), 5337-8
SC 33 (Carbohydrates)
DT J
CO JACSAT
PY 1968
LA Eng
AN CA70(1):4503j
AB 2′,3′-O-Isopropylideneuridine is treated with dicyclohexylcarbodiimide and Me2SO in the presence of pyridinium trifluoroacetate to give I (R = uracil moiety) (II). II and I (R = adenine moiety) are treated with PH3P:CHP(O)(OPh)2 to give III which are reduced to 5′-deoxy-5′-(phosphinylmethyl)nucleosides (IV), where R1 is Ph, PhCH2, and H. The IV (R1 = H) are hydrolyzed to give V.
IT 7307-92-8P 22257-12-1P 22257-13-2P 22257-14-3P
22257-15-4P
(prepn. of)

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AN CA64:15973f
DT P
IT 7292-42-4 7307-92-8 7533-93-9

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